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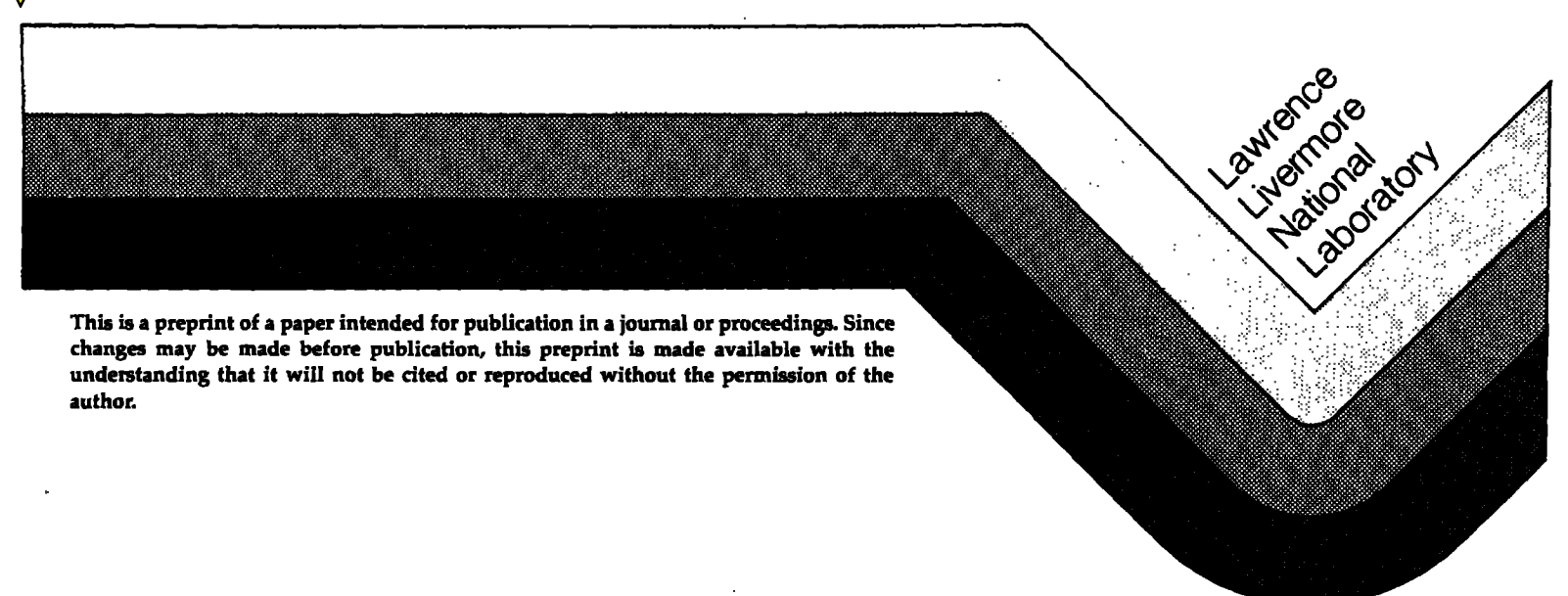

Interactions Between a Laminar Flame and End Gas Autoignition

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Abstract

A numerical model combining one dimensional fluid mechanics and detailed chemical kinetics is used to examine the interactions between laminar flame propagation and end gas autoignition at high temperatures and pressures of approximately 30 atmospheres. The flame is found to have very little influence on the computed rates of fuel-air autoignition in the end gas, but the subsequent high rate of heat release during autoignition is shown to produce strong acoustic waves in the burned gases. The effects of temperature fluctuations in the end gas on the locations at which autoignition is initiated is also investigated numerically.

INTRODUCTION

Increases in the costs of petroleum fuels in recent years have created a need to improve fuel economy of internal combustion engines. This can be achieved by increasing the compression ratio of the engine, but such increases are severely limited by the onset of engine knock. Environmental concerns have necessitated the virtual elimination of the most effective metal-based antiknock additives such as tetraethyl lead (TEL), resulting in a great deal of interest in finding effective alternative methods of controlling engine knock. However, a more thorough understanding of the physics and chemistry of the autoignition process is needed before significant progress in this complex area can be achieved.

One technique that recently has been applied to the autoignition problem is that of detailed numerical modeling of the chemical kinetics of hydrocarbon fuel ignition [1-4]. These models use experimentally observed temperatures, pressures, and fuel-air mixture ratios from typical automobile engines to predict the time required for the unburned fuel-air mixture (the so-called "end gas") to ignite spontaneously. If the time required for self-ignition is relatively long, then there is usually sufficient time for this end gas to be consumed by the conventional flame front in the engine prior to autoignition, and knocking is avoided. However, if the autoignition occurs rapidly, then there is the possibility that some fraction of the end gas will ignite before it is consumed by the flame front, resulting in knocking conditions. This overall approach has

demonstrated some success in describing part of the engine knock problem, including the ability to reproduce the time of knock occurrence and variations in tendency to knock with temperature, pressure, residence time, and fuel-air equivalence ratio. Furthermore, this approach has also helped to identify the most important parts in the mechanism by which metal-based antiknock additives such as TEL slow the autoignition process and reduce the tendency of engines to knock [1]. However, there are still many questions which remain pertaining to both the physical and chemical processes occurring in knocking engines.

When knock occurs, its most immediate manifestation is the onset of a distinct sound signal, a "ringing" from the engine. This response is a result of interactions between fluid mechanical motions within the engine chamber and the metal components of the engine. There has been a great deal of discussion as to the exact nature of these fluid motions in the engine chamber, including how they are generated by the autoignition of the end gas and whether or not shock waves are present. The present paper represents an attempt to address some of these questions under highly idealized conditions.

Previous modeling efforts [1,4] using the HCT code [5] have focused on the autoignition of the end gas, dealing only with a homogeneous medium that effectively neglected fluid mechanical motions with the reacting gas mixture. The compression and heating of the end gas resulting both from piston motion and from flame propagation in the combustion chamber were included in the model as externally applied boundary conditions. Aside from this formulation of the boundary conditions, there was no way to examine the fluid mechanical coupling between the burned gas and the end

gas. However, there are two major mechanisms by which this coupling can take place, one dealing with the influence of the burned gases on the rate of autoignition, and the second dealing with the generation of pressure inhomogeneities within the combustion chamber by the autoignition of the end gas. Within the limitations of the present model, both types of fluid mechanical coupling are considered in the present paper.

Flame propagation and heat transfer in actual engines take place under highly turbulent conditions. Unfortunately, current abilities to simulate detailed chemical kinetics and flame propagation in turbulent environments are still very limited. In contrast, these processes can be simulated quite accurately and completely under laminar conditions. The problem selected for study therefore was that of an end gas igniting in the presence of a flame front and burned combustion products, all taking place under laminar conditions. The possible relevance of the computed results to conditions in a turbulent engine are then discussed.

NUMERICAL MODEL AND CHEMICAL KINETIC MECHANISM

Numerical calculations were carried out using the HCT computer code [5] which solves the coupled conservation equations of mass, momentum, energy and each chemical species. The thermal diffusivity and molecular diffusivities are based on a simplified treatment of the general multicomponent diffusion problem and are discussed in a previous paper [6]. The fuels considered were propane and n-butane; the reaction mechanism has been described in detail elsewhere [7,8], and for space limitations the rate parameters will not be included here.

For each fuel, the reaction mechanism consists of two principal submechanisms. The first part is a high temperature mechanism which has been shown [7,8] to reproduce combustion rates, ignition delays, and intermediate species concentrations in shock tubes, laminar flames, and the turbulent flow reactor. The temperature regime covered by these experiments is approximately 900K - 2000K. For each fuel, a second submechanism has been included which describes the fuel oxidation in a lower temperature range, from approximately 550K - 900K. The lower temperature range is characterized by different major reaction paths than those encountered at higher temperatures, with the addition of molecular oxygen to various alkyl radicals being the most important feature. The application of the current model to combustion in the lower temperature range, and the resulting refinements of the reaction mechanism to reproduce experimental data, are described elsewhere [9,10]. The model accurately describes low temperature hydrocarbon oxidation, including the region of negative temperature coefficient and the behavior of "cool flames", while the high temperature submechanism correctly reproduces the processes associated with hot ignition and flame propagation. The two submechanisms merge together smoothly, so as the temperature is increased from 550K to 1500K there is a continuous transition from one set of dominant reactions to another.

Homogeneous gas phase chemical kinetics calculations, in which the fluid motions were neglected, have been reported previously [1,4]. In the current model computations, a one dimensional domain is considered, in which the majority of the combustible mixture has already been burned. In

most of the calculations, the linear extent of the combustion chamber is 4 cm. A laminar flame is propagating towards the combustion chamber boundary, with an unreacted "end gas" between the flame and the wall. The fuel fraction and gas temperature in a typical case are shown in Figure 1. At this particular time, the flame is located at a distance of approximately 0.4 mm from the wall of the combustion chamber. The end gas is at a temperature of about 1100 K, and there is a thermal boundary layer caused by heat transfer to the wall which is maintained at 400 K.

The simultaneous processes of end gas autoignition and laminar flame propagation were then calculated, while several of the most important parameters were varied in order to examine their relative importance. In some of the calculations, heat transfer from the reacting end gas to the colder wall is included, in order to assess the relative importance of heat losses in the autoignition rate. In another series of calculations, the relative timing of the flame arrival and time of autoignition were changed, ranging from a condition in which no autoignition occurred to one in which as much as 20% of the total fuel-air mixture was consumed by the autoignition. The fuel-air equivalence ratio, the fuel type and molecular structure, and the temperature-pressure history in the combustion chamber were also varied. In addition, the influence of spatial inhomogeneities in the end gas was examined.

For all of the model calculations, an initial combustion chamber pressure of 30 atmospheres was assumed. End gas initial temperatures were 1000 K, and wall temperatures of 400 K and 1000 K were used. All of these parameters were chosen to approximate thermodynamic conditions in end gases of reciprocating engines.

RESULTS

The most immediate conclusion reached in these calculations was that the presence of the flame in the combustion chamber has relatively little direct influence on the autoignition of the end gas. Of course, the continuing heat release and pressure increase produced by the flame continue to compress and heat the end gas, and this does increase the rate of autoignition. However, transport of heat and radical species from the flame were found to have essentially no effect on the autoignition. These transport processes, which are the central features of flame propagation, really have an effect only over a spatial range which is usually referred to as the flame thickness or the diffusion length. Beyond that distance, the end gas does not "see" the flame itself, although it "feels" the flame through the compressional work done by the flame. In the computed model results for cases in which autoignition occurred, the autoignition time for a given sample of end gas was found to be the same, regardless of whether or not a flame was present. A sequence of temperature profiles in this regime is shown in Figure 2. The ignition of the end gas is quite uniform, although heat transfer to the wall and from the flame contribute to some degree of nonuniformity. In this case the autoignition of the end gas is promoted by a reduction in the rate of heat transfer to the cold wall (the wall temperature was maintained at 1000 K, rather than 400 K as in the case shown in Fig. 1).

In those cases in which the time for consumption by the flame was substantially shorter than the time for autoignition, the presence of the flame did not accelerate the autoignition process. This case is illustrated by the temperature profiles in Figure 3. Here the autoignition

is retarded by the enhanced heat transfer to the colder wall at 400 K. The two extremes represented by Figures 2 and 3 are clearly very distinguishable. Furthermore, the time scales for the two cases are quite different, with the flame propagation process being slower than the more abrupt autoignition event of Figure 2.

In the transition regime in which the two time scales were comparable, the combustion occurred as a composite event which actually looked very much like an accelerated flame [11]. A series of spatial plots of temperature in the end gas region are presented in Figure 4 for this intermediate regime. If an equivalent "flame position" is defined as the point at which the gas temperature is 2000 K, then it is clear from Fig. 4 that the "flame" is accelerating as the end gas ignites. However, this is not actually a flame, since the advancing temperature front is not the product of transport processes as in a conventional flame, but rather an artifact of the simultaneous processes of ignition and flame propagation.

This result has two significant implications. First, it appears that the same conclusion should apply to turbulent combustion in an automotive engine chamber. Under turbulent conditions, the analogous flame thickness is of course significantly larger, since the turbulent transport coefficients are larger than the laminar values. However, beyond the turbulent flame thickness, the turbulent flame should have little or no influence on the autoignition rate of the end gas. The second implication of the above result, which should also apply to the turbulent case, is that since the flame and end gas regions are effectively decoupled, modeling of end gas ignition should easily be incorporated into most engine combustion models as a simple "satellite" submodel. This supports the approach taken in a number of existing submodels of engine knock [12,13].

In those cases in which autoignition of the end gas occurs, the calculations indicate that significant pressure gradients can be produced within the combustion chamber. This results from the fact that the rate of heat release in the igniting end gas is larger than the rate of dissipation of the pressure gradients by convective heat and mass transfer. These pressure gradients then generate large gas velocities within the combustion chamber. In some of the cases examined, these velocities were as high as 150 m/s, 15% of the sound speed in the burned gases. An example of this pattern is presented in Figure 5, with both the pressure and gas velocity profiles shown. These pressure waves travel back and forth across the combustion chamber at the local sound speed, eventually decaying. However, these waves have both the frequency and magnitude to be identified with the ringing sound which is associated with engine knock. That is, the relevant parameters in this system are the relative rates of heat release in the end gas as compared with the rate of propagation of sound waves, both of which should be approximately the same in laminar and in turbulent regimes. Neither the rate of flame propagation nor the flame thickness appear to play any significant role, at least in those cases in which end gas autoignition does take place. Therefore, these results show that the autoignition of the end gas does have a significant effect on the post-ignition motions of the burned gases in the combustion chamber.

In the past, there have been speculations that engine knock might be the result of actual detonation in the end gas, reactive shock waves initiated by the autoignition of a significant fraction of the fuel-air charge. Although the current computations indicate that autoignition can generate strong acoustic waves, there is no indication that anything resembling actual detonation waves would be produced, consistent with recent experimental observations [4].

A third set of calculations was carried out to examine the possible influence of temperature and density fluctuations in the end gas. As shown in Figures 2-4, the temperature profile in the end gas is essentially a monotonic function of position, so long as the only processes included are flame propagation and a thermal boundary layer. However, autoignition in actual combustion chambers is often identified as occurring at specific sites which vary from cycle to cycle. Under the turbulent conditions in which this takes place, another factor which may have some influence is the existence of turbulent fluctuations in the end gas. Since these fluctuations are stochastic in nature, they will occur at different locations in the engine chamber on different cycles. If it could be shown that such fluctuations can lead to the existence of preferred sites for autoignition, then this could explain the experimental observations of seemingly random locations at which engine knock is initiated.

In this series of calculations, the reacting end gas region is artificially perturbed by introducing temperature fluctuations of varying magnitude and spatial extent. An increase in local temperature produces an enhanced rate of autoignition, but the competing processes of thermal conduction and thermal diffusion act to dissipate the fluctuation. The model helped to identify critical values for the properties of the fluctuations, above which the fluctuation provided a preferred site for autoignition and below which the entire end gas region ignited as a whole.

SUMMARY

These computations represent an attempt to couple a sophisticated chemical kinetics treatment of end gas autoignition with a reasonably detailed treatment of gas phase fluid mechanics. The model has examined several problems in which this coupling may be important. It was found that although the flame in the combustion chamber does not have a significant direct influence on the rate of end gas autoignition, the autoignition can generate pressure waves in the burned gases which are quite large. Generalizations of these results, in which only laminar flames were considered, to turbulent conditions were discussed. Since the important parameters in these results are usually relative rates of different processes, the conclusions reached here should be applicable to engine conditions, as long as the turbulent flame parameters and time scales are used for comparisons. These conclusions tend to support the logic used in the construction of knock submodels in engine combustion models in current use. It also suggests that it would be relatively simple to incorporate autoignition rates, computed using very detailed chemical kinetic mechanisms, into existing engine combustion models.

ACKNOWLEDGMENTS

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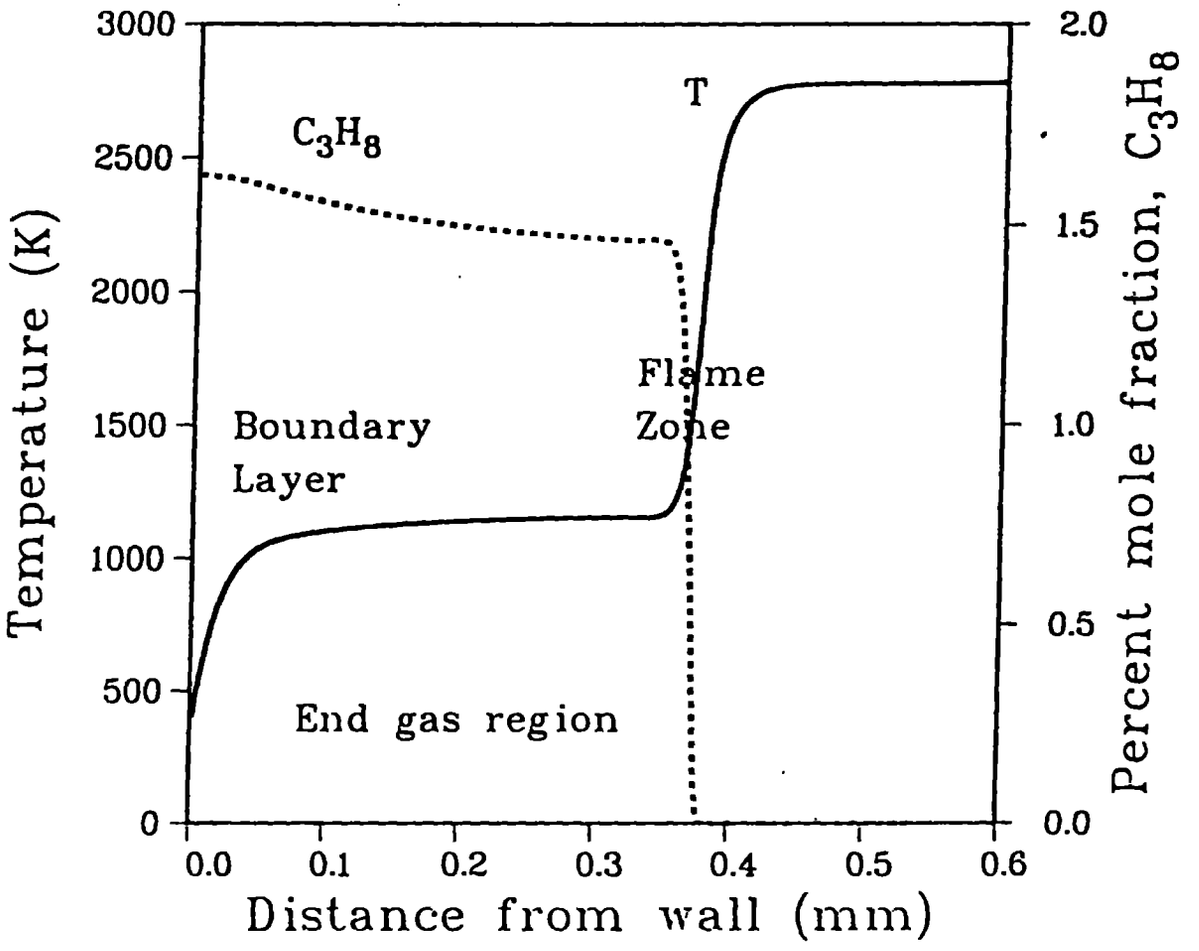

Figure 1. Schematic diagram of flame-end gas configuration, showing spatial variations of temperature and fuel concentration. The thermal boundary layer is also indicated.

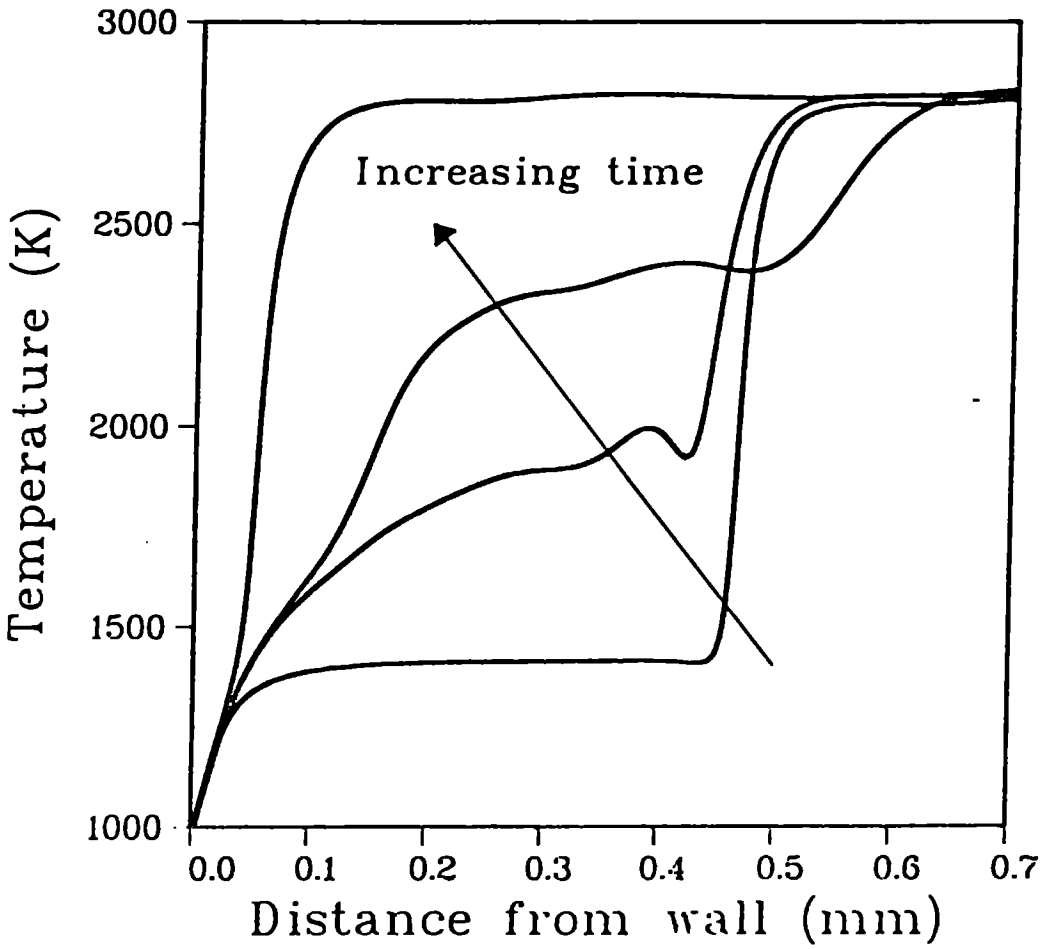

Figure 2. History of the spatial temperature profile with a wall temperature of 1000 K. The end gas undergoes autoignition prior to flame arrival.

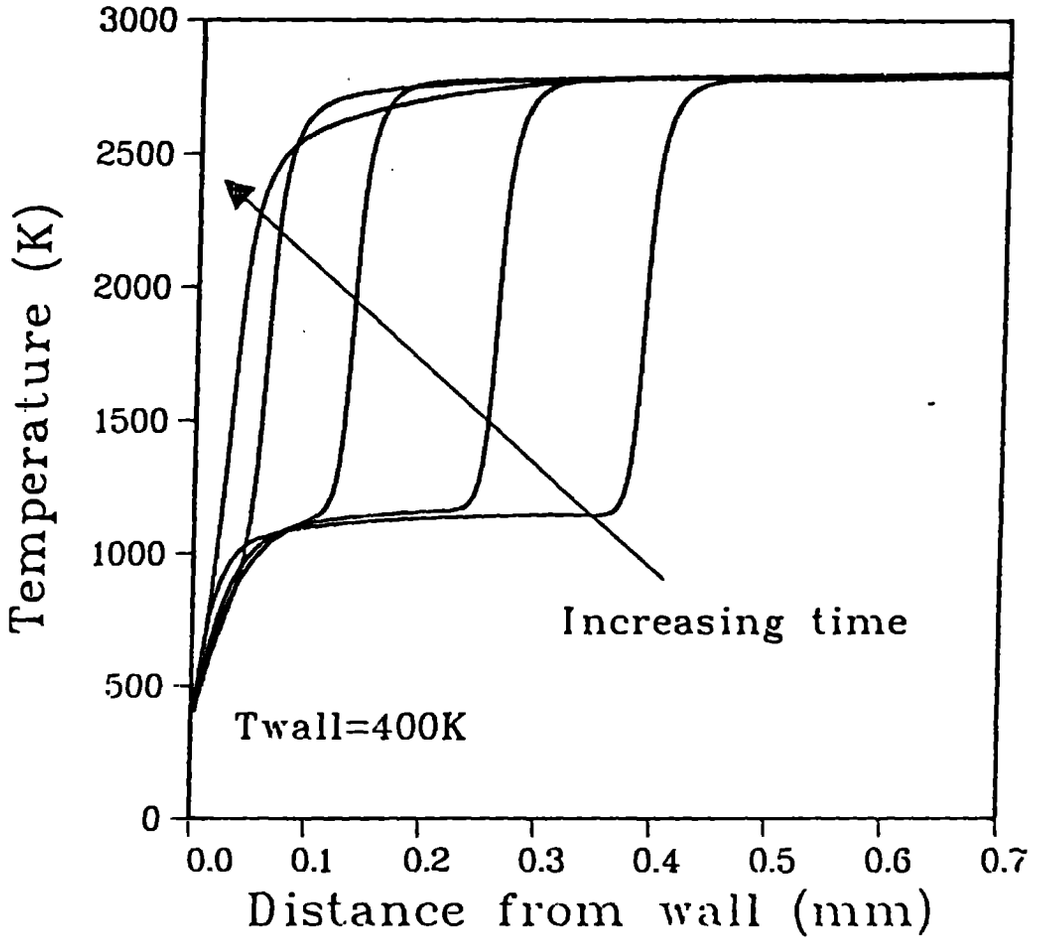

Figure 3. History of the spatial temperature profile with a wall temperature of 400 K. No end gas autoignition occurs.

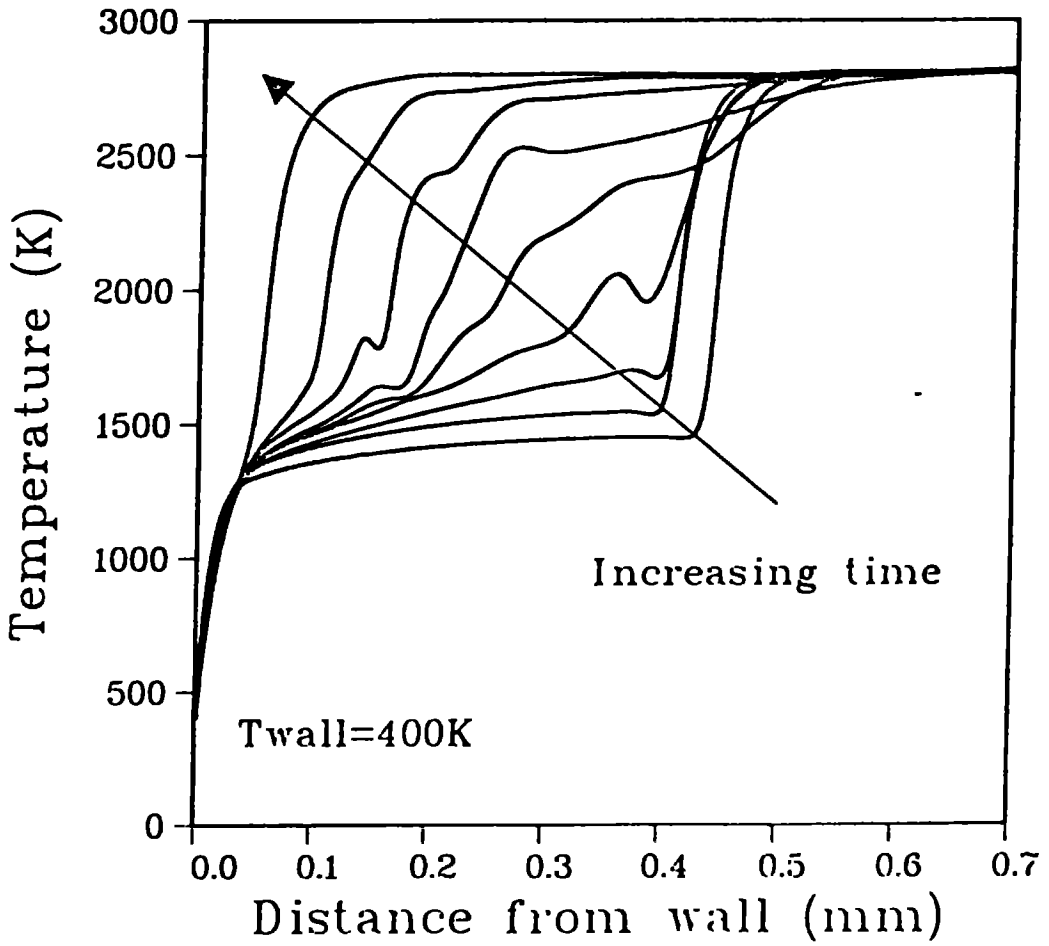

Figure 4. History of the spatial temperature profile in the intermediate situation, with autoignition occurring on the same time scale as flame arrival.

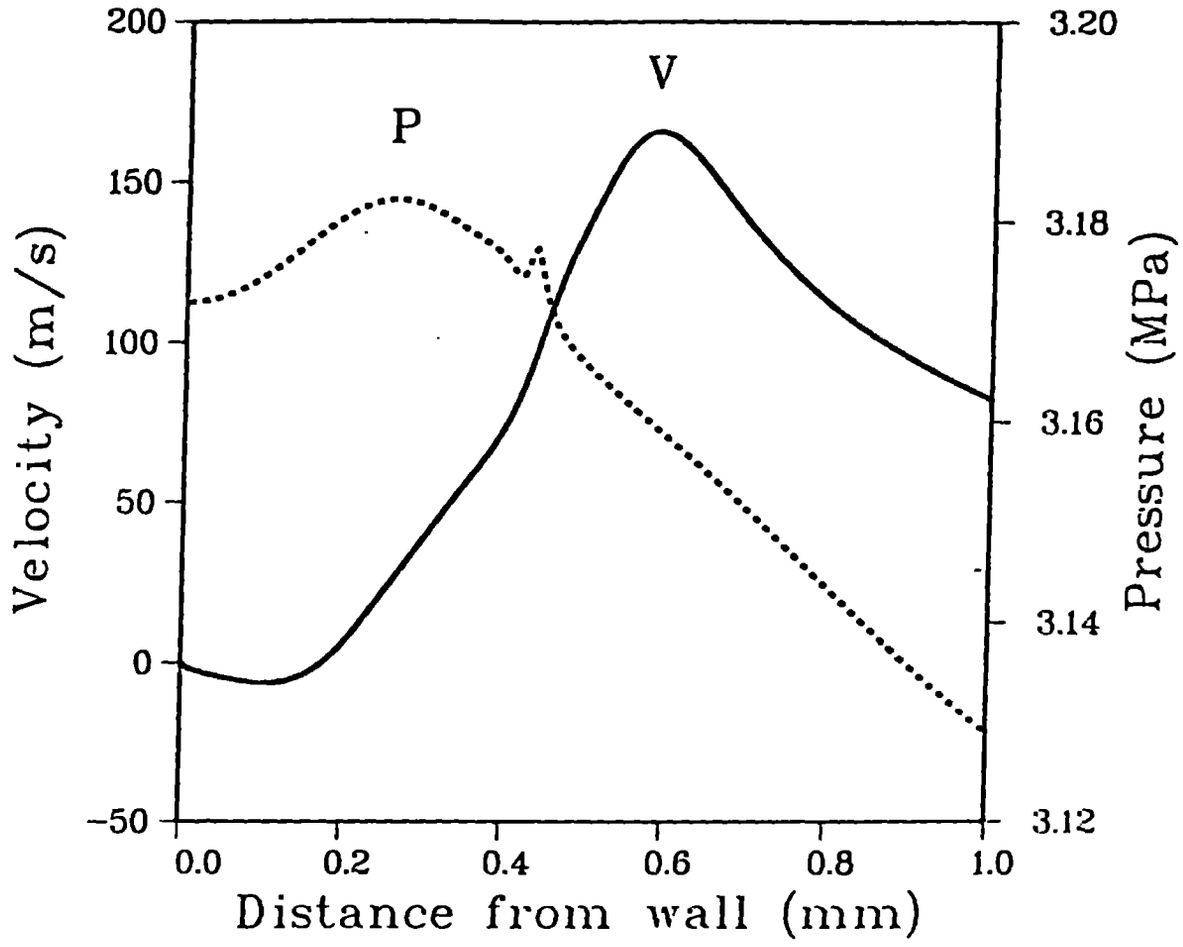

Figure 5. Pressure and velocity profiles shortly after autoignition has occurred.